

Optical and DC conductivity in the $d=2$ Hubbard model Including Vertex Corrections

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arXiv:1101.4037



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Calculating transport properties



A few things we know about resistivity

- From Bloch-Boltzmann theory
 - T^2 for Fermi-liquid
 - T for AFM QCP in $d=2$ (Moriya 1990)
 - T^2 with cold spots (Hlubina-Rice 1995)
- From Mott-Ioffe-Regel (wave nature)
 - Maximum metallic resistivity
- From DMFT
 - Limit can be exceeded with linear T (Palsson, Kotliar 2001)



Mott-Ioffe-Regel limit

$$\sigma = \frac{ne^2\tau}{m}$$

$$n = \frac{k_F^2}{2\pi d}$$

$$\ell = v_F\tau$$

$$k_F\ell = 1$$

$$\sigma_{MIR} = \frac{1}{d} \frac{e^2}{h}$$



Vertex corrections

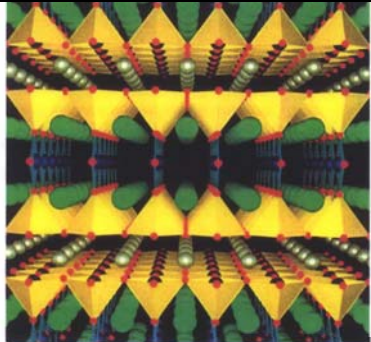
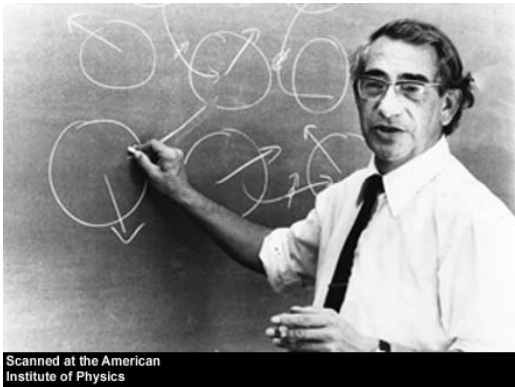
- Single particle excitations (ARPES) measures single particle scattering rate
- Resistivity measurement: particle-hole pair
 - Lifetime counts (self-energy)
 - Interaction between excited particle and hole counts (vertex correction)
 - The two must be evaluated in a consistent way (Ward identities)



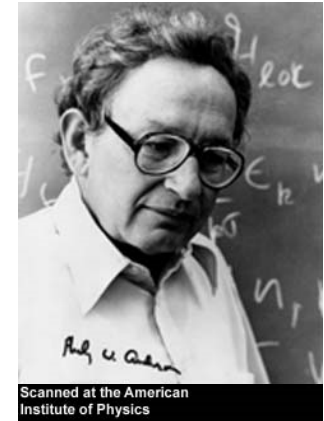
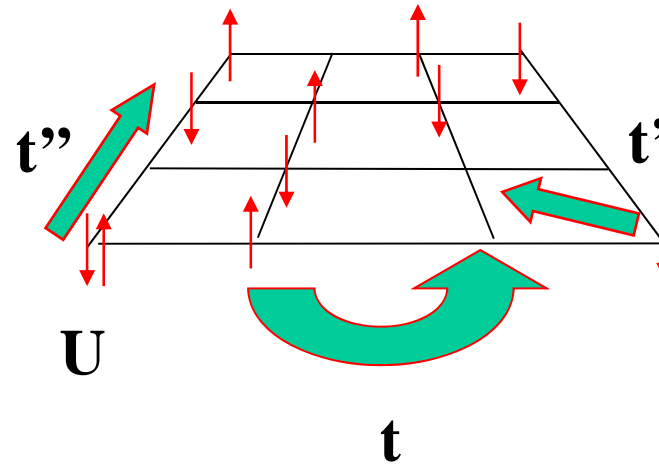
The model

The Hubbard model

Simplest microscopic model for *Cu O* planes.



High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.
 $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ 92-37



$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

No mean-field factorization for d-wave superconductivity

Weak to intermediate coupling

T. Moriya, Y. Takahashi, and K. Ueda, Journal of the Physical Society of Japan, **59**, 2905 (1990/08).

R. Hlubina and T. Rice, Physical Review B (Condensed Matter), **51**, 9253 (1995/04/01).

A. Rosch, Phys. Rev. Lett., **82**, 4280 (1999).

H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys., **79**, 1015 (2007).

S. Wernbter and L. Tewordt, Phys. Rev. B, **48**, 10514 (1993).

T. Dahm, L. Tewordt, and S. Wernbter, Physical Review B (Condensed Matter), **49**, 748 (1994/01/01).

H. Kontani, Journal of the Physical Society of Japan, **76**, 074707 (2007/07).

H. Kontani, K. Kanki, and K. Ueda, Physical Review B (Condensed Matter), **59**, 14723 (1999/06/01).

Y. Yanase, Journal of the Physical Society of Japan, **71**, 278 (2002/01/).

H. Kontani, Reports on Progress in Physics, **71**, 026501 (2008/02/).

H. Maebashi and H. Fukuyama, Journal of the Physical Society of Japan, **66**, 3577 (1997/11/).

H. Maebashi and H. Fukuyama, Journal of the Physical Society of Japan, **67**, 242 (1998/01/).

Boltzmann

Boltzmann disordered

T-matrix

FLEX

FLEX with MT-VC

Review

Vertex within FL



Strong coupling

F. Mancini and A. Avella, *Advances in Physics*, **53**, 537 (2004).

T. A. Maier, *ArXiv Condensed Matter e-prints* (2003), arXiv:cond-mat/0312447.

M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, *Phys. Rev. B*, **61**, 12739 (2000).

K. Haule and G. Kotliar, *Physical Review B (Condensed Matter and Materials Physics)*, **76**, 104509 (2007).

K. Haule and G. Kotliar, *Europhysics Letters*, **77**, 6 pp. (2007/01/), ISSN 0295-5075.

N. Lin, E. Gull, and A. J. Millis, *Phys. Rev. B*, **80**, 161105 (2009), arXiv:0909.1625 [cond-mat.str-el].

S. Okamoto, D. Sénéchal, M. Civelli, and A.-M. S. Tremblay, *Phys. Rev. B*, **82**, 180511 (2010).

Composite operators

Quantum cluster no vertex

DCA, with vertex



Methodology

Weak to intermediate
coupling approaches



Two-Particle Self-Consistent TPSC



TPSC: general ideas

- General philosophy
 - Drop diagrams
 - Impose constraints and sum rules
 - Conservation laws
 - Pauli principle ($\langle n_{\sigma}^2 \rangle - \langle n_{\sigma} \rangle$)
 - Local moment and local density sum-rules
- Get for free:
 - Mermin-Wagner theorem
 - Kanamori-Brückner screening
 - Consistency between one- and two-particle $\Sigma G = U \langle n_{\sigma} n_{-\sigma} \rangle$

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);

Theoretical methods for strongly correlated electrons also (Mahan, 3rd)



TPSC equations

$$\chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U_{sp}\chi_0(q)}$$

$$\langle (n_{\uparrow} - n_{\downarrow})^2 \rangle = \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle - 2\langle n_{\uparrow}n_{\downarrow} \rangle \quad \frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2\langle n_{\uparrow}n_{\downarrow} \rangle$$

$$U_{sp} = U \frac{\langle n_{\uparrow}n_{\downarrow} \rangle}{\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle} \quad \text{Kanamori-Brückner screening}$$

$$\Sigma_{\sigma}^{(2)}(k) = Un_{\bar{\sigma}} + \frac{U}{8} \frac{T}{N} \sum_q \left[3U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q) \right] G_{\sigma}^{(1)}(k+q)$$

Does not assume Migdal. Vertex at same level of approximation as G

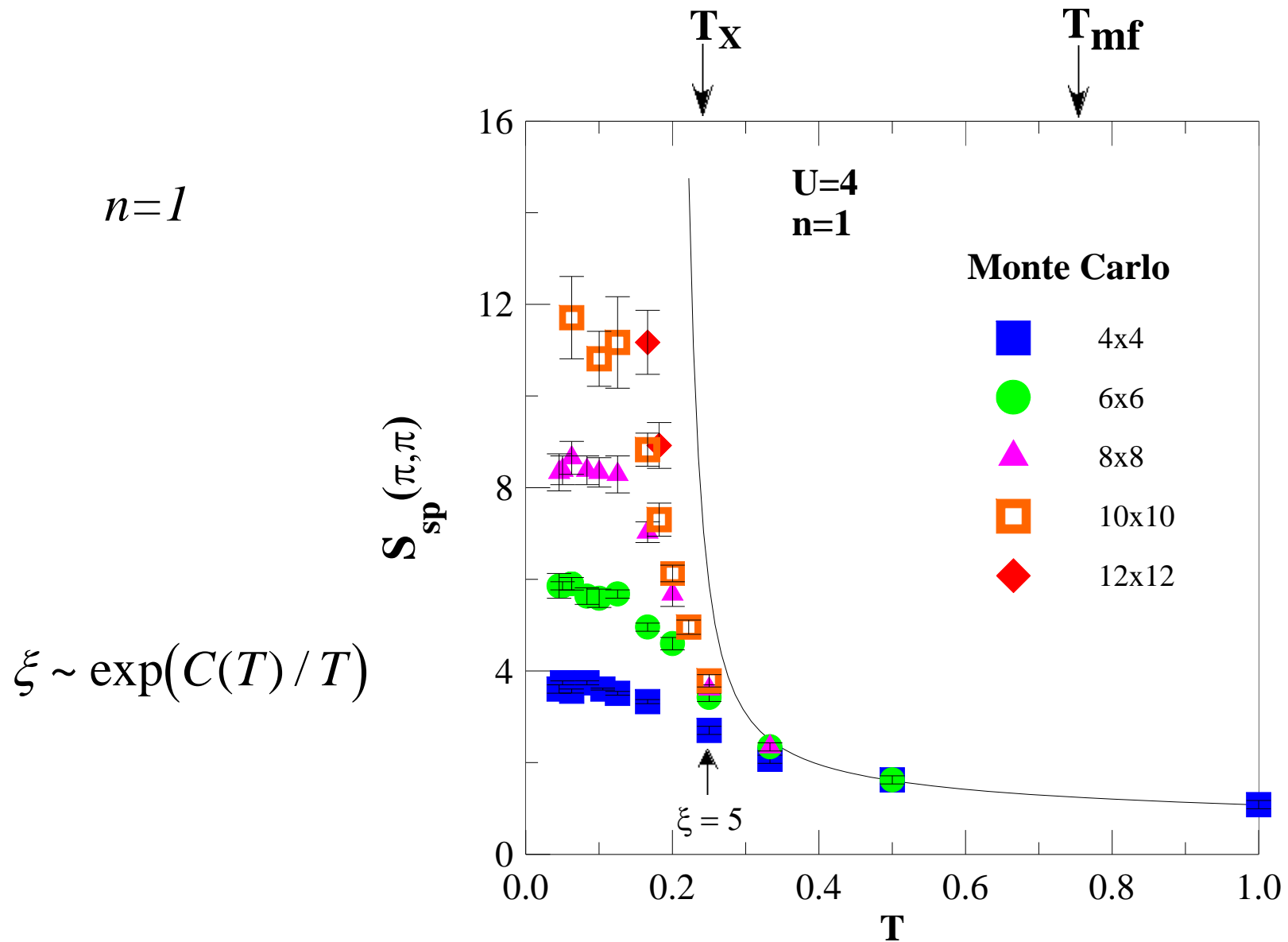
Internal accuracy check

$$\frac{1}{2} \text{Tr} \left(\Sigma^{(2)} G^{(1)} \right) = U \langle n_{\uparrow}n_{\downarrow} \rangle = \frac{1}{2} \text{Tr} \left(\Sigma^{(2)} G^{(2)} \right)$$



Benchmark TPSC with Quantum Monte Carlo





Calc.: Vilk et al. P.R. B **49**, 13267 (1994)

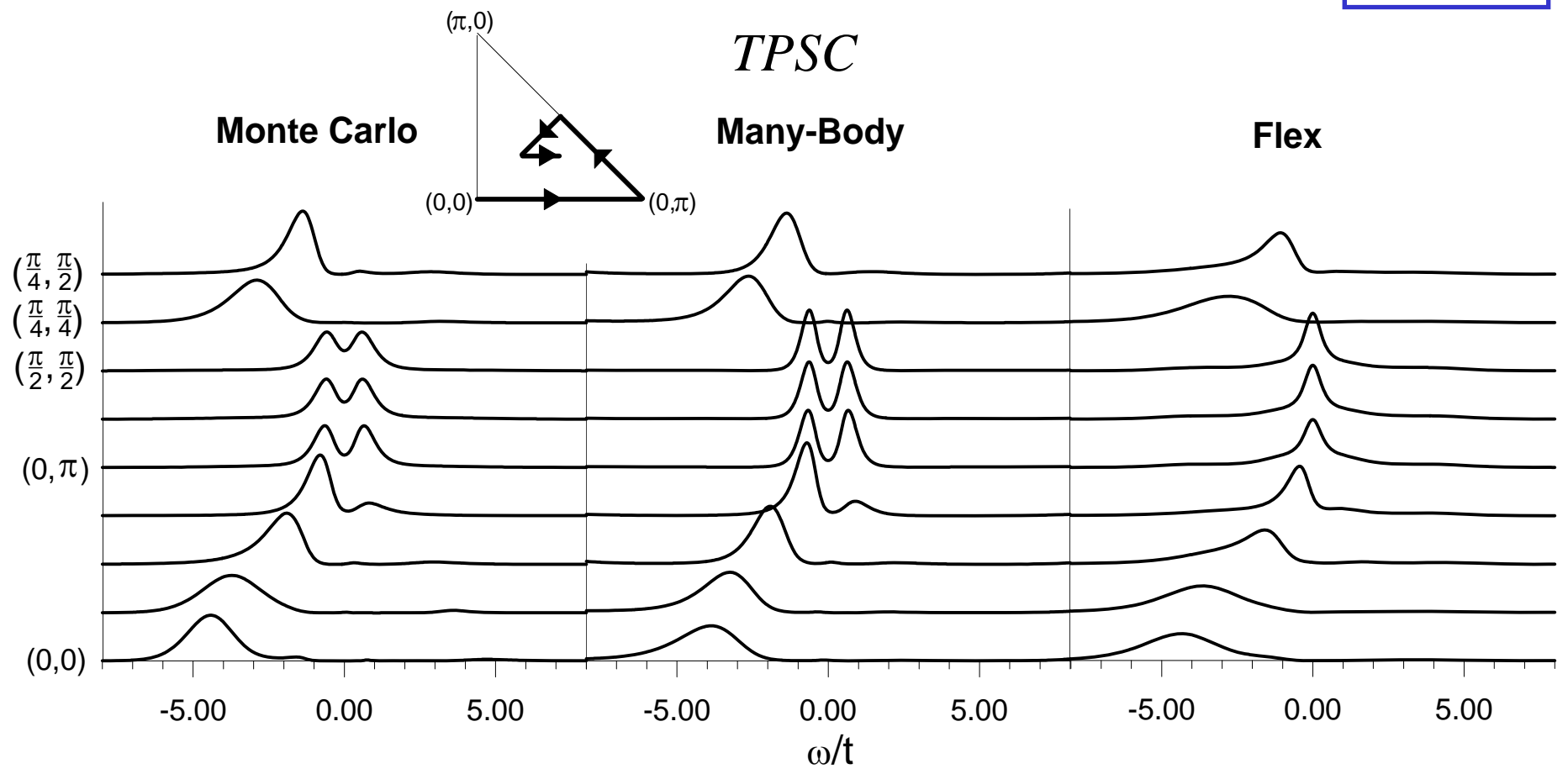
QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

$O(N = \infty)$ A.-M. Daré, Y.M. Vilk and A.-M.S.T Phys. Rev. B **53**, 14236 (1996)

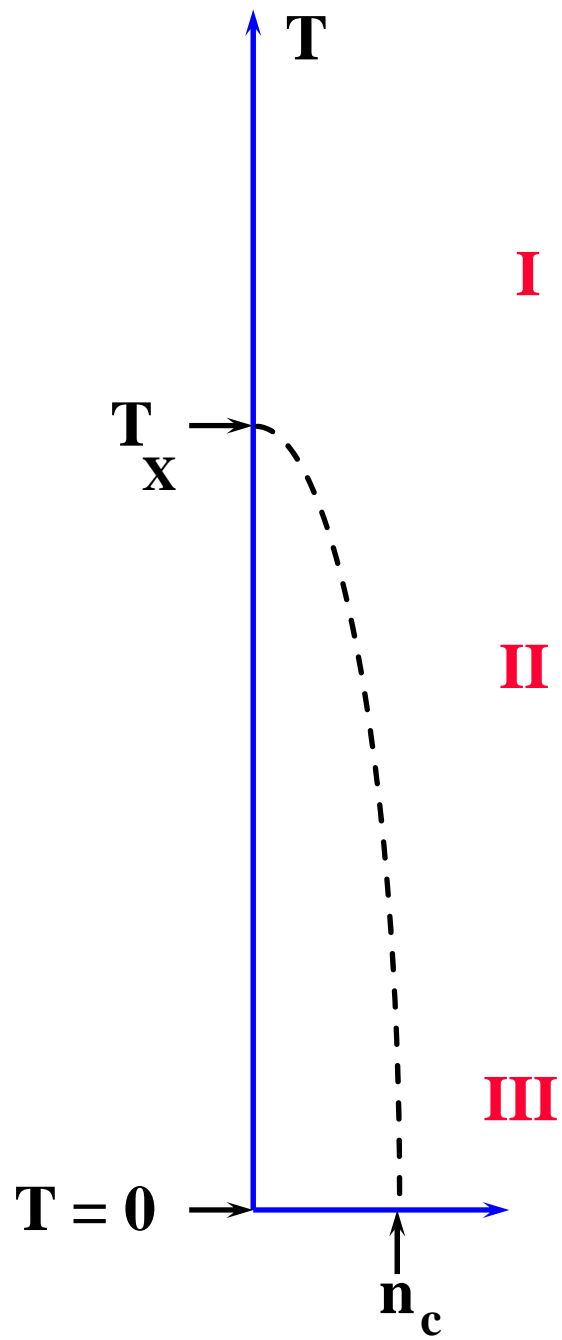


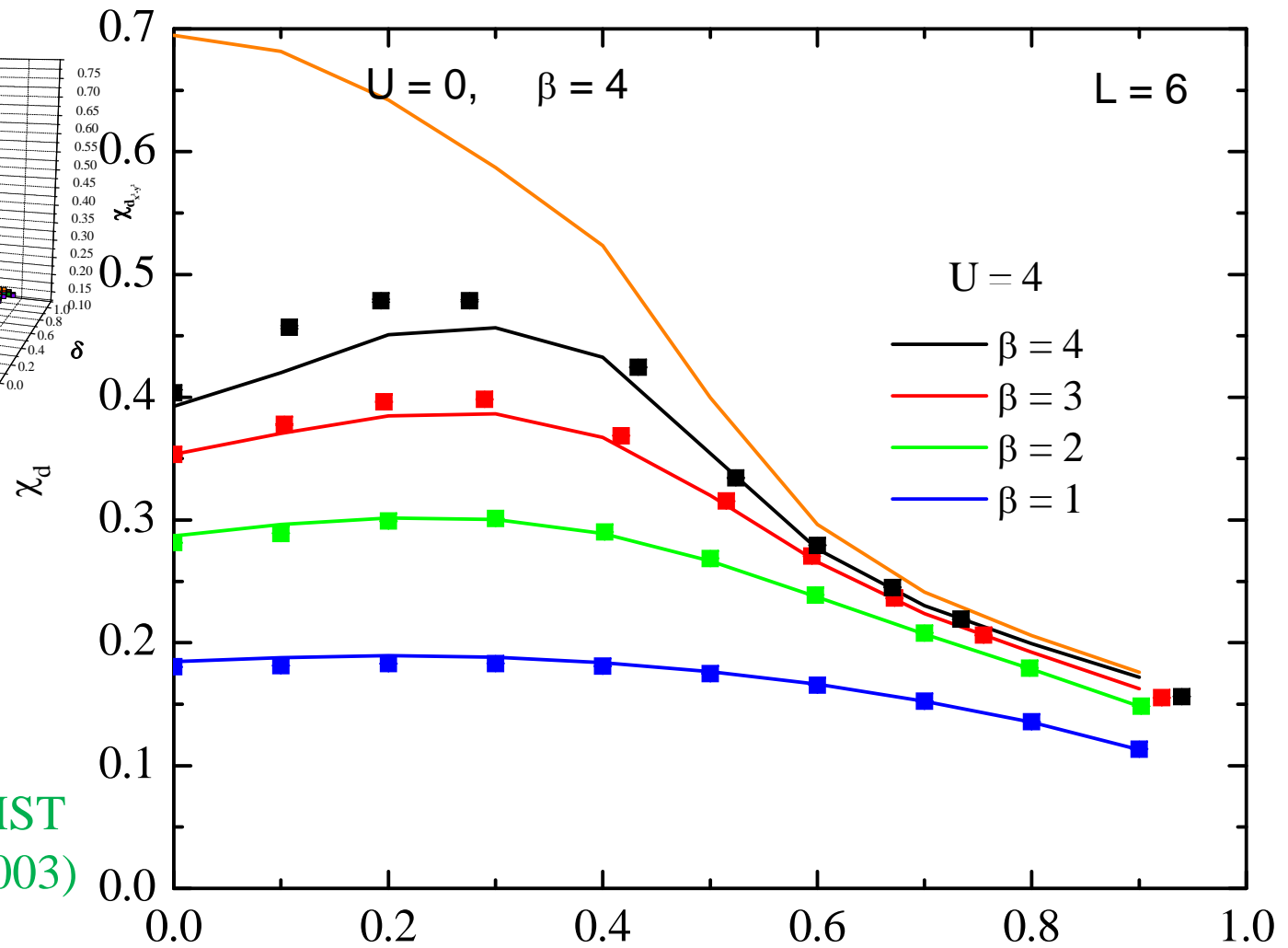
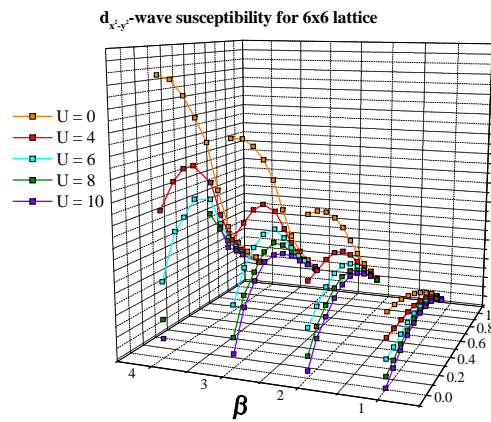
Proofs...

$U = +4$
 $\beta = 5$



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).





Kyung, Landry AMST
PRB **68**, 174502 (2003)

QMC: symbols.
Solid lines analytical.

Doping
Kyung, Landry, A.-M.S.T.



The pseudogap in electron-doped cuprates



Analytically :

effect of critical fluctuations on particles (RC regime)

$$\hbar\omega_{sf} \ll k_B T$$

Imaginary part: compare Fermi liquid, $\lim_{T \rightarrow 0} \Sigma_R''(\mathbf{k}_F, 0) = 0$

$$\Sigma_R''(\mathbf{k}_F, 0) \propto \frac{T}{v_F} \int d^{d-1} q_{\perp} \frac{1}{q_{\perp}^2 + \xi^{-2}} \propto \frac{T}{v_f} \xi^{3-d} \propto \frac{\xi}{\xi_{th}}$$

$$\Delta \varepsilon \approx \nabla \varepsilon_{\mathbf{k}} \cdot \Delta \mathbf{k} \approx v_F \hbar \Delta k = k_B T$$

$$\text{Im} \Sigma^R(\mathbf{k}_F, 0) \propto -U \xi / \left(\frac{\xi}{\xi_{th}} \xi_0^2 \right) > 1$$

Why leads to pseudogap

$$A(\mathbf{k}, \omega) = \frac{-2\Sigma_R''}{(\omega - \varepsilon_{\mathbf{k}} - \Sigma_R')^2 + \Sigma_R''^2}$$

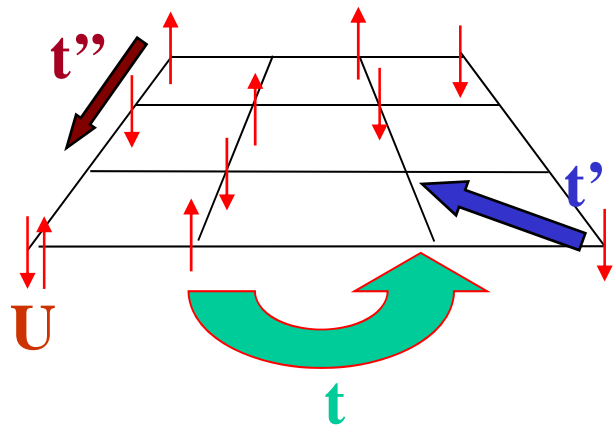
Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);



Parameters for electron-doped near optimal δ

$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

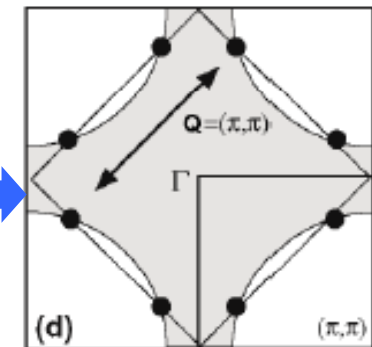


$$U = 6t$$

fixed

$$t' = -0.175t, t'' = 0.05t$$

$$t = 350 \text{ meV}, T = 200 \text{ K}$$



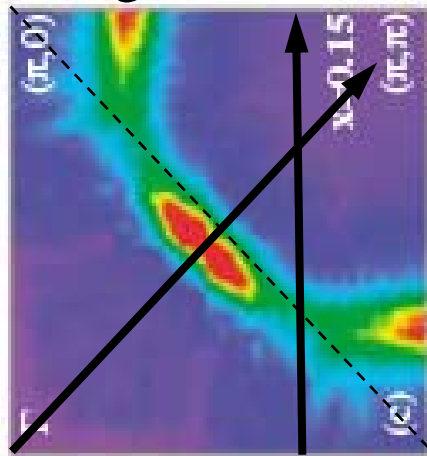
Weak coupling $U < 8t$

$n = 1 + x$ – electron filling

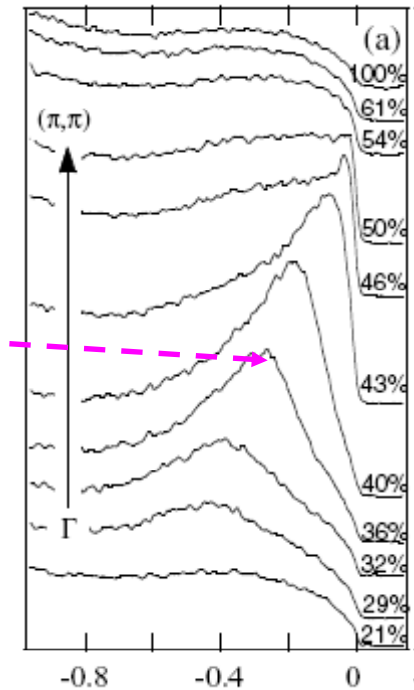
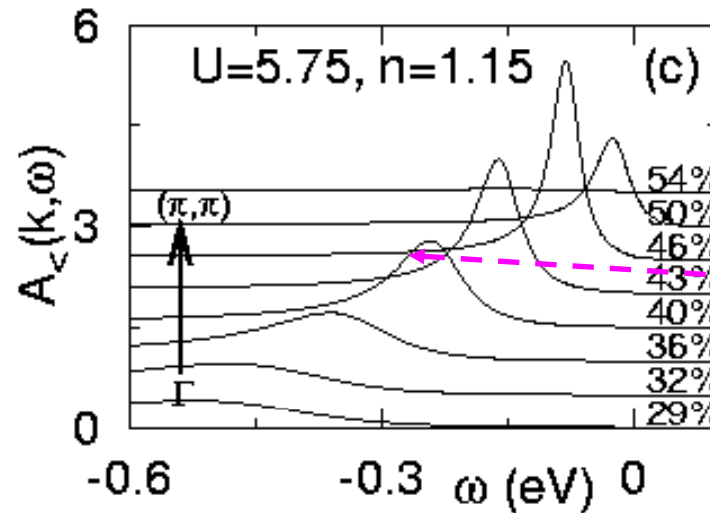


15% doped case: EDCs in two directions

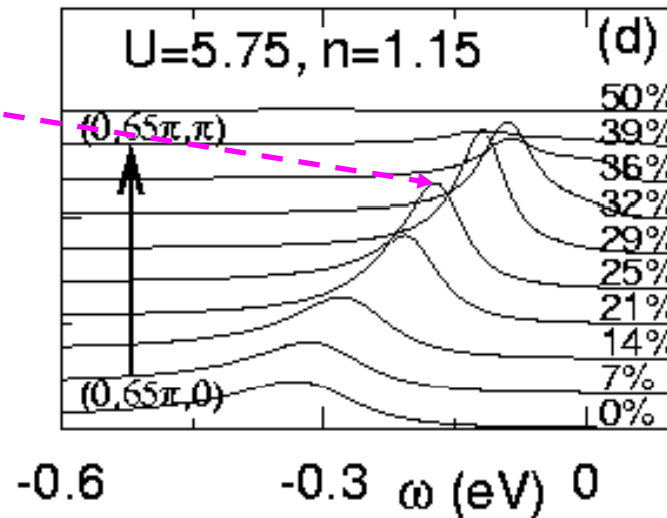
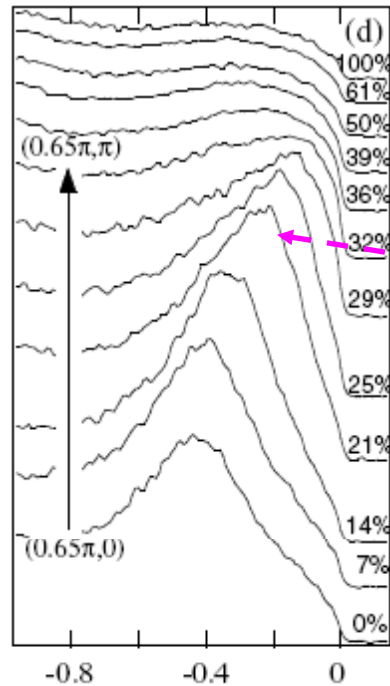
Armitage et al. PRL 2001



TPSC



Exp

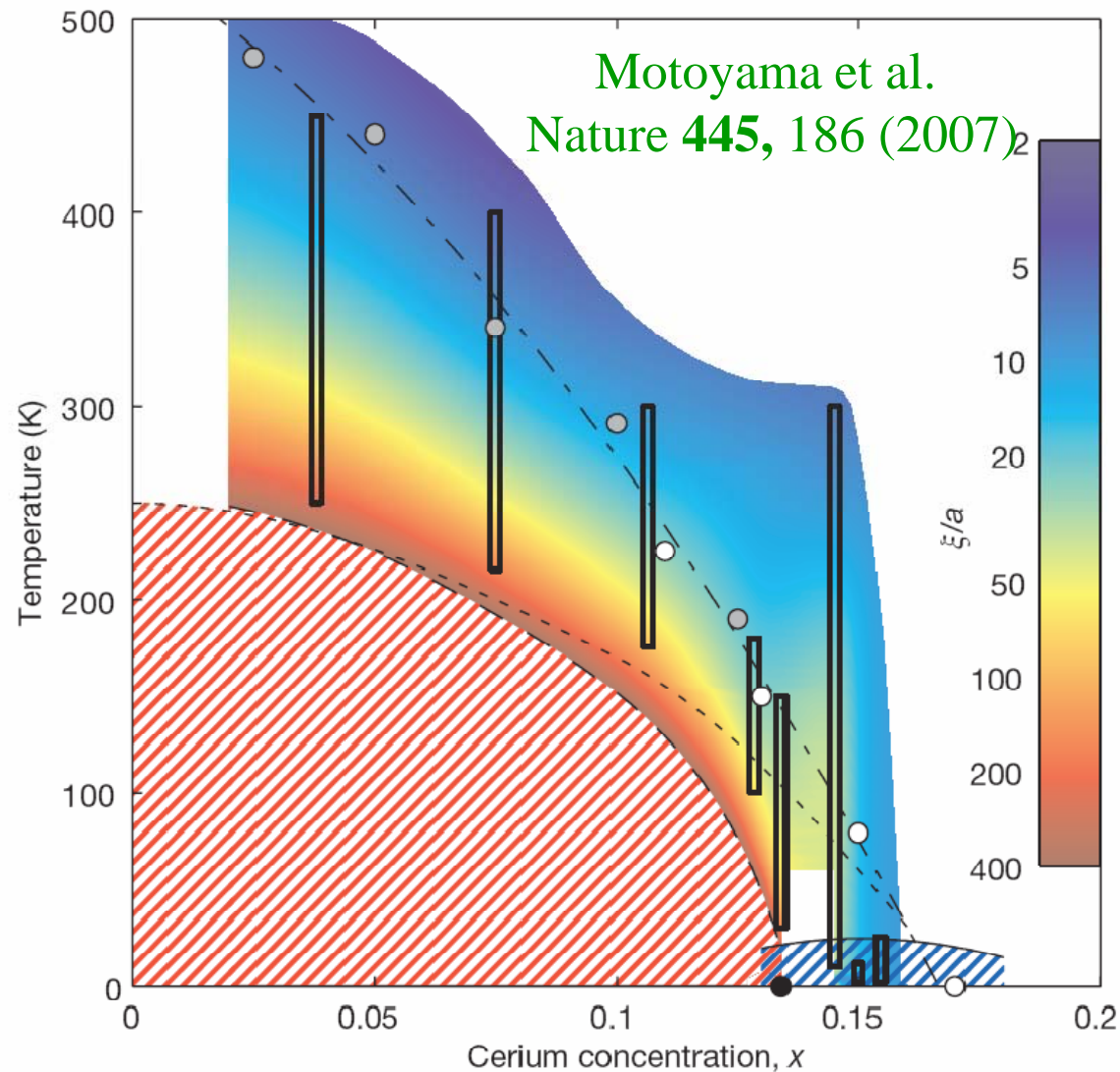


Exp

Hankevych, Kyung,
A.-M.S.T., PRL (2004).



Electron doped Neutron scattering



$$\xi^* = 2.6(2)\xi_{th}$$

Vilk, A.-M.S.T (1997)

Kyung, Hankevych,
A.-M.S.T., PRL, sept.
2004

Semi-quantitative fits of
both ARPES and
neutron

Precursor of SDW state (dynamic symmetry breaking)

- Y.M. Vilks and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769-1771 (1995).
- Y. M. Vilks, Phys. Rev. B 55, 3870 (1997).
- J. Schmalian, *et al.* Phys. Rev. B **60**, 667 (1999).
- B.Kyung *et al.*, PRB **68**, 174502 (2003).
- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
- R. S. Markiewicz, cond-mat/0308469.





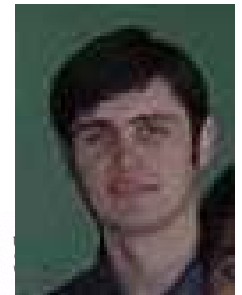
Dominic Bergeron

Calculation of the conductivity

Bumsoo Kyung



Vasyl Hankevych



Linear response : No quasiparticle assumption

- ▶ Linear response theory:

$$\boxed{\text{Re } \sigma_{xx}(\omega) = \frac{\chi''_{j_x j_x}(\omega)}{\omega}}$$

- ▶ $\chi_{j_x j_x}(q_x, \omega)$ is the *current-current* correlation function:

$$\chi_{j_x j_x}(\mathbf{r} - \mathbf{r}', t - t') = \frac{\delta \langle j_x(\mathbf{r}, t) \rangle}{\delta A_x(\mathbf{r}', t')} = i \langle [j_x(\mathbf{r}, t), j_x(\mathbf{r}', t')] \rangle \theta(t - t')$$

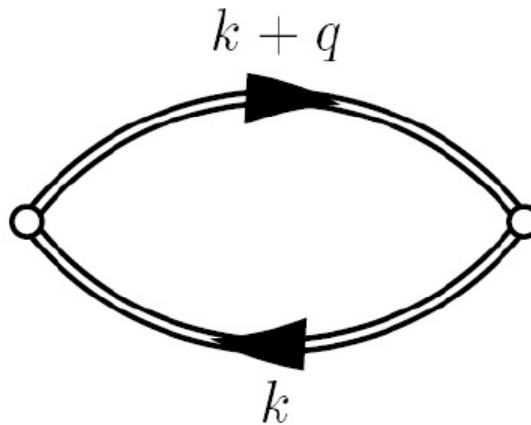
- ▶ $\chi_{j_x j_x}$ can be calculated with vertex corrections obtained from

$$\left. \frac{\delta U_{sp}}{\delta A_x} \right|_{A_x=0, \mathbf{q}=0} = \left. \frac{\delta U_{ch}}{\delta A_x} \right|_{A_x=0, \mathbf{q}=0} = 0$$

$$\boxed{\frac{\delta \Sigma^{(2)}}{\delta A_x}}$$

Bubble

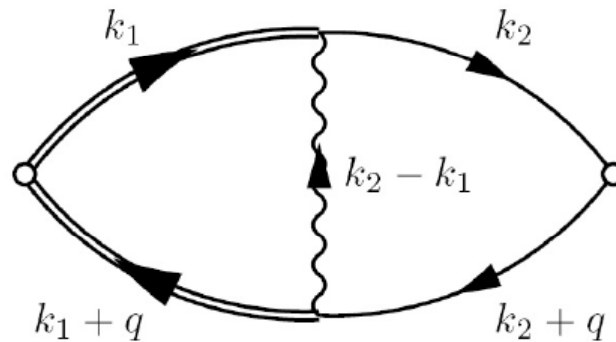
$$\chi_{j_x j_x}^b(iq_n, \mathbf{q} = 0) = -\frac{2T}{N} \sum_k \left(\frac{\partial \varepsilon_k}{\partial k_x} \right)^2 G^{(2)}(k) G^{(2)}(k + iq_n)$$



Maki Thomson

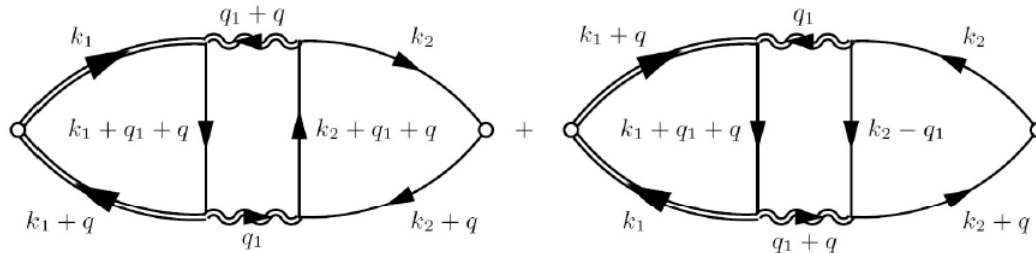
$$\chi_{j_x j_x}^{vc1}(iq_n) = -\frac{U}{4} \left(\frac{T}{N}\right)^2 \sum_{k_1 k_2} G^{(2)}(k_1) G^{(2)}(k_1 + iq_n) G^{(1)}(k_2) G^{(1)}(k_2 + iq_n)$$

$$\frac{\partial \varepsilon_k}{\partial k_x}(k_1) \frac{\partial \varepsilon_k}{\partial k_x}(k_2) [3U_{sp} \chi_{sp}(k_2 - k_1) + U_{ch} \chi_{ch}(k_2 - k_1)]$$



Aslamasov-Larkin

$$\begin{aligned} \chi_{j_x j_x}^{vc2}(iq_n) = & \frac{U}{2} \left(\frac{T}{N} \right)^3 \sum_{k_1, k_2, q_1} \frac{\partial \varepsilon_k}{\partial k_x}(k_1) \frac{\partial \varepsilon_k}{\partial k_x}(k_2) G^{(2)}(k_1) G^{(2)}(k_1 + iq_n) \\ & \times G^{(1)}(k_2) G^{(1)}(k_2 + iq_n) \left[G^{(1)}(k_2 + q_1 + iq_n) + G^{(1)}(k_2 - q_1) \right] \\ & \times G^{(1)}(k_1 + q_1 + iq_n) \left(3U_{sp} \frac{1}{1 - \frac{U_{sp}}{2} \chi_0(q_1)} \frac{1}{1 - \frac{U_{sp}}{2} \chi_0(q_1 + iq_n)} \right. \\ & \left. + U_{ch} \frac{1}{1 + \frac{U_{ch}}{2} \chi_0(q_1)} \frac{1}{1 + \frac{U_{ch}}{2} \chi_0(q_1 + iq_n)} \right) \end{aligned}$$



Dominic Bergeron

3 loops : at 10 Gflops, $T=0.01 t$

400 billion years for 100 frequencies

Fast Fourier transforms



Analytical continuation

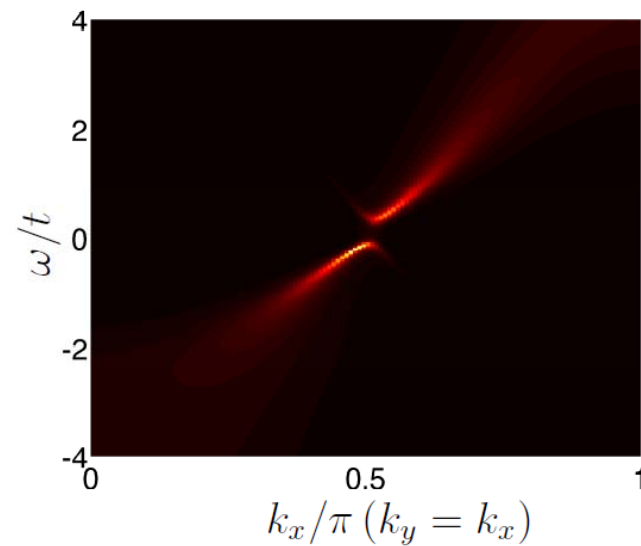
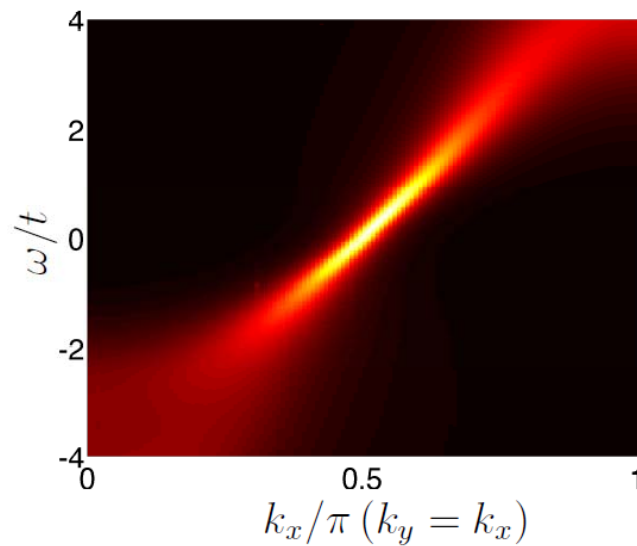
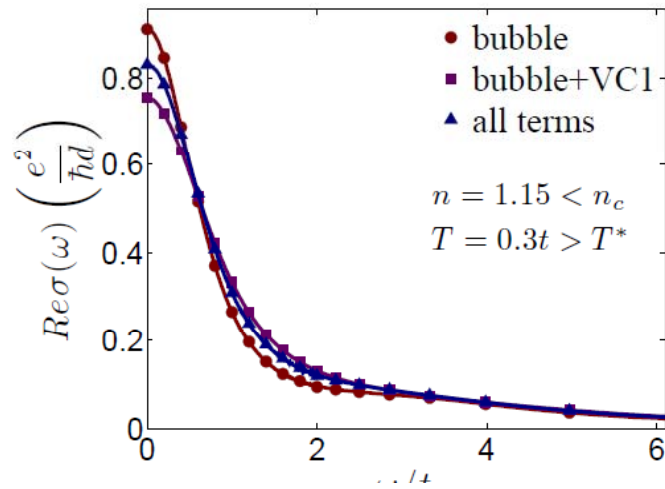
- Analytical continuation of Matsubara conductivity
 - For 10^{-6} precision, Padé not enough
 - Maximum Entropy
 - Checked with model spectral densities



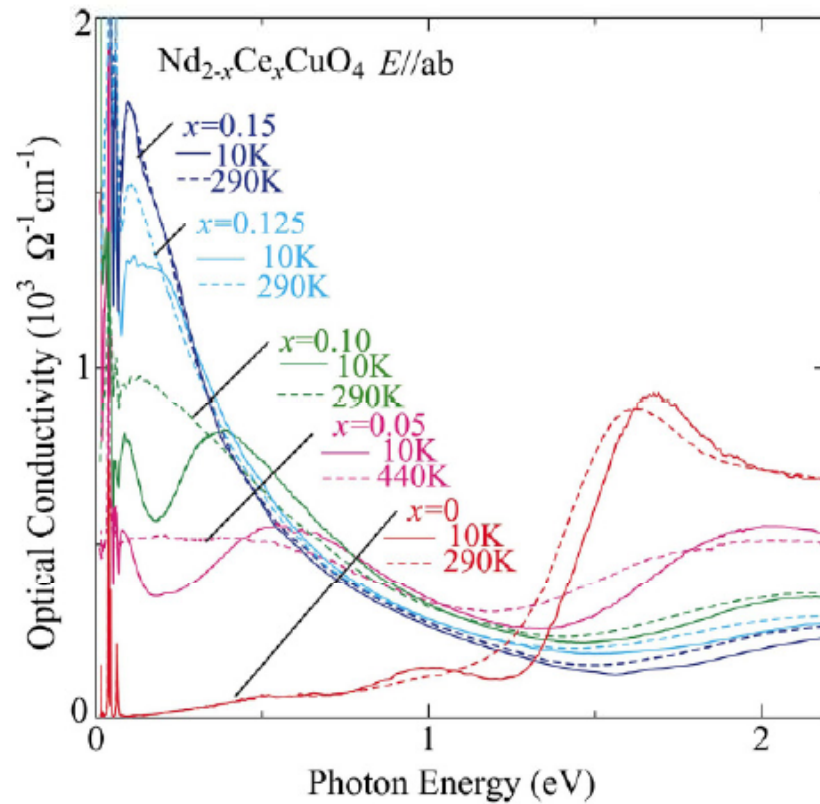
Optical conductivity

Optical conductivity $n < n_c$

$$U = 6t, t' = -0.175t, t'' = 0.05t$$



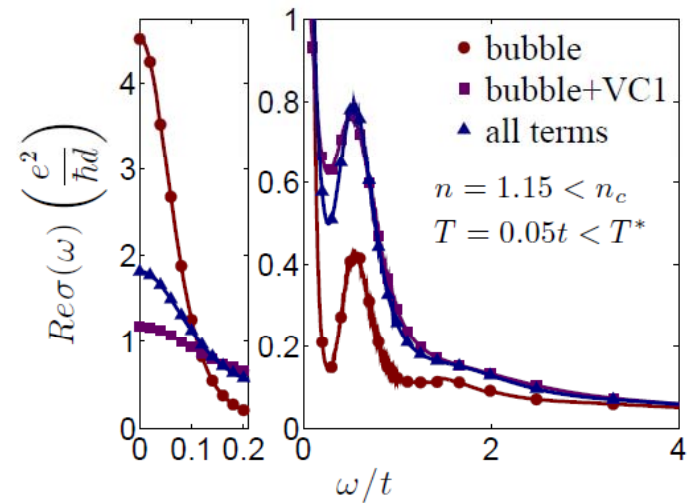
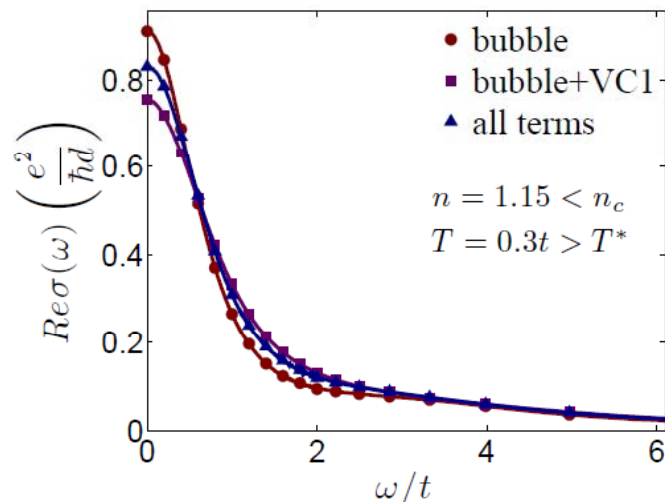
Optical conductivity in NCCO



Y. Onose *et al.*, Phys. Rev. B, 69, 24504 (2004)

Optical conductivity $n < n_c$ and $n > n_c$

$$U = 6t, t' = -0.175t, t'' = 0.05t$$



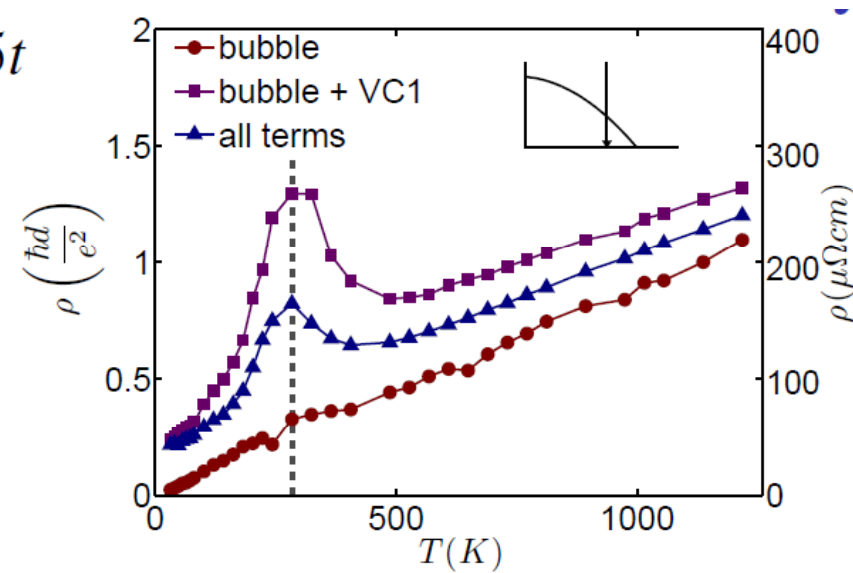
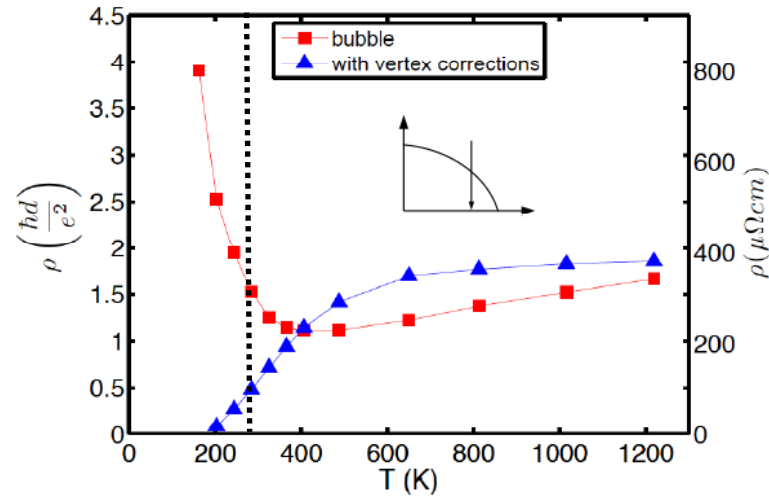
Results : DC resistivity

Entering the pseudogap

$$U = 6t, t' = -0.175t, t'' = 0.05t$$

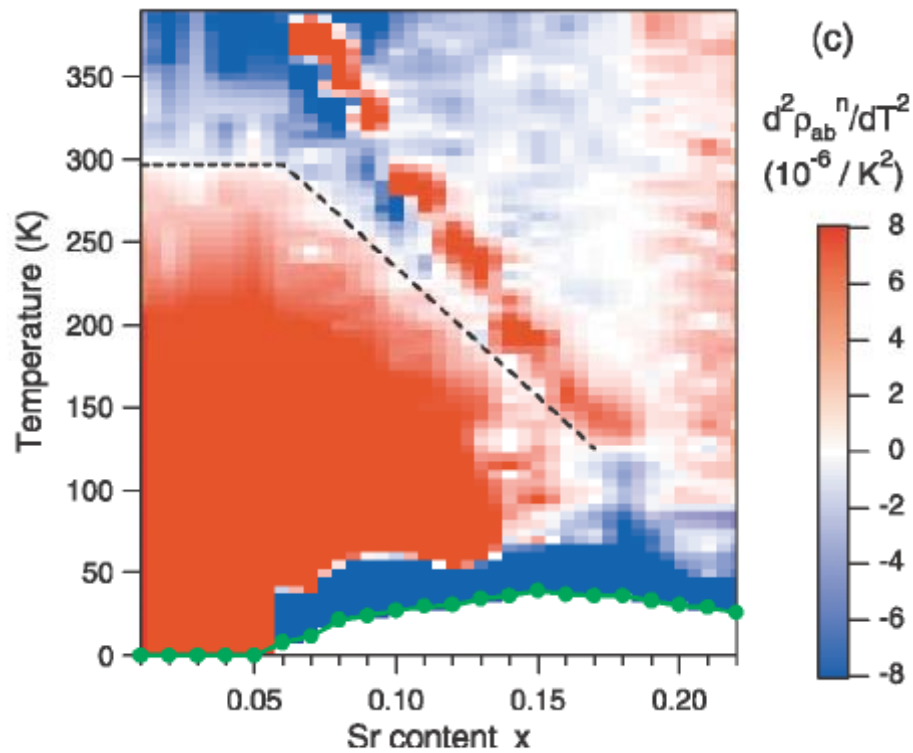
$$U = 6t, t' = 0$$

$$p = 0.15$$

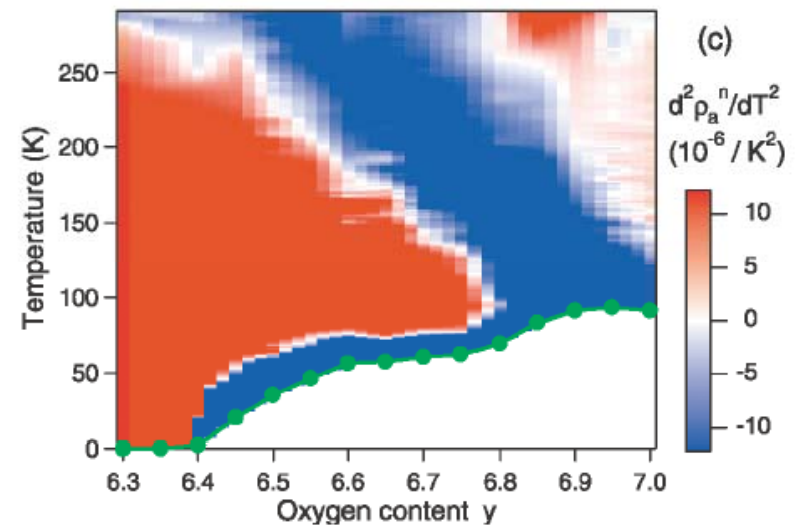


$$(t = 0.35eV \text{ and } d = 5\text{\AA})$$

Curvature maps



LSCO

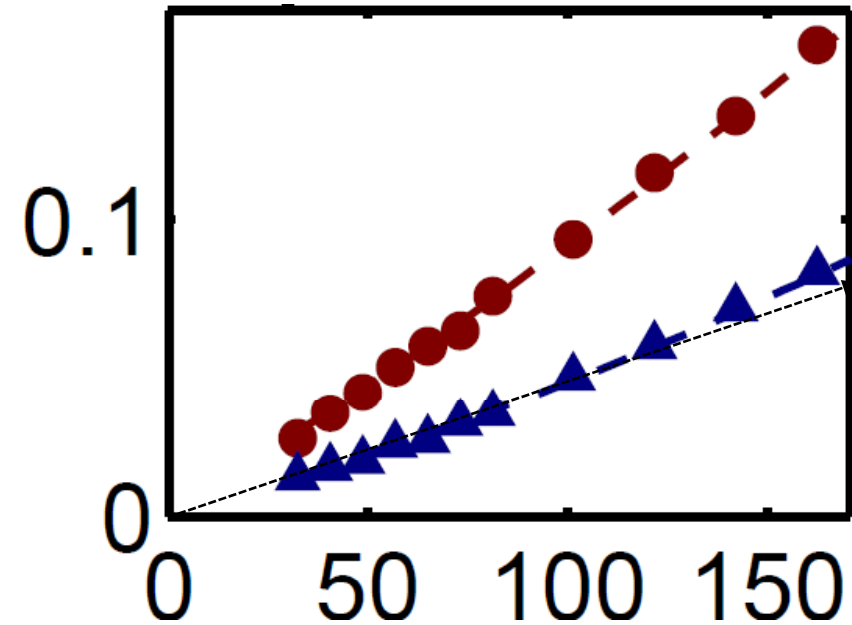
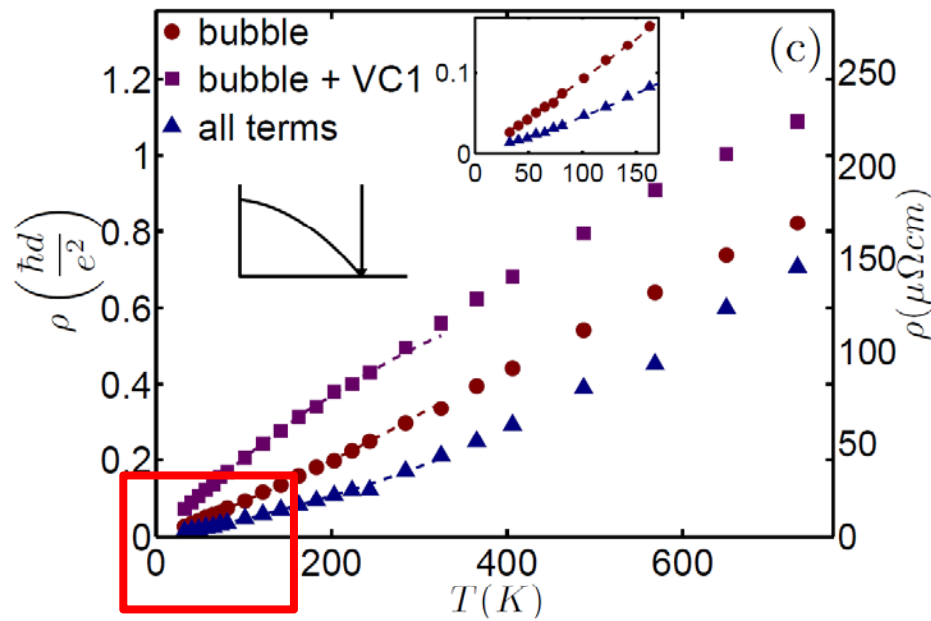


YBCO

Ando et. Al. PRL **93**, 267001 (2004)

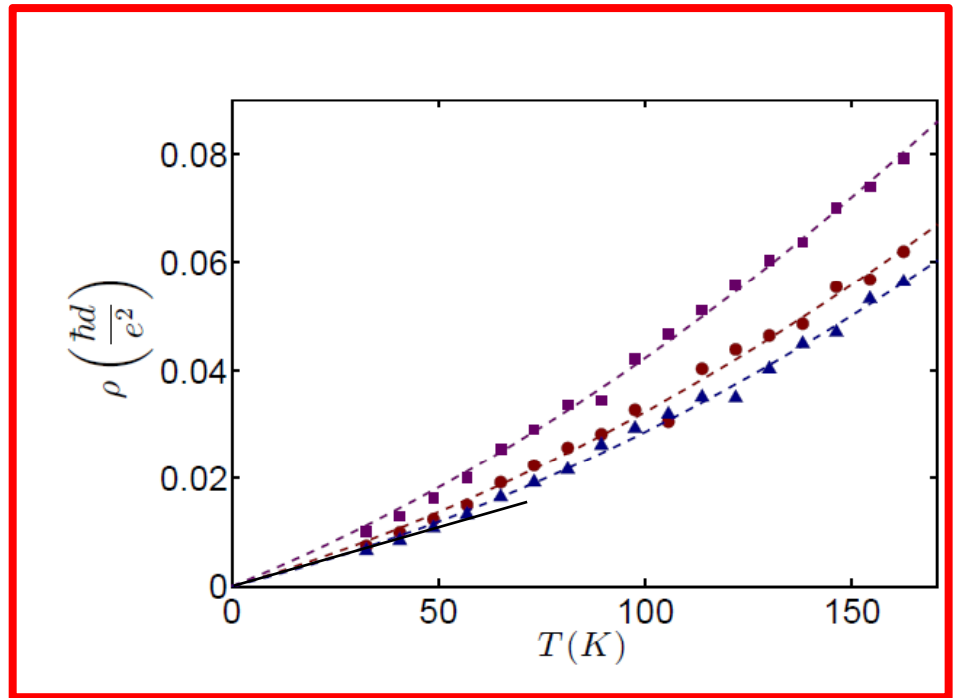
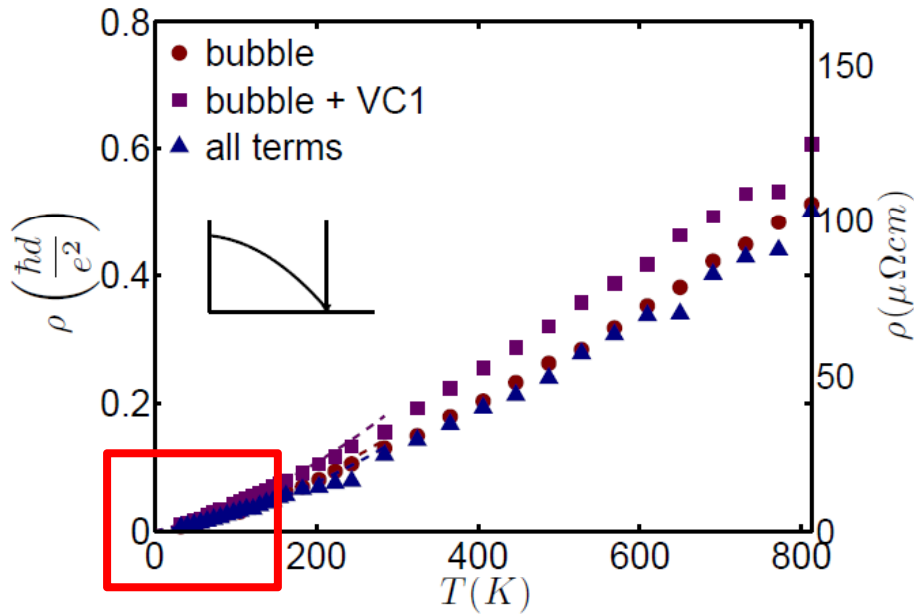
At the quantum critical point

$$U=6t, t'=0$$



At the QCP for finite t'

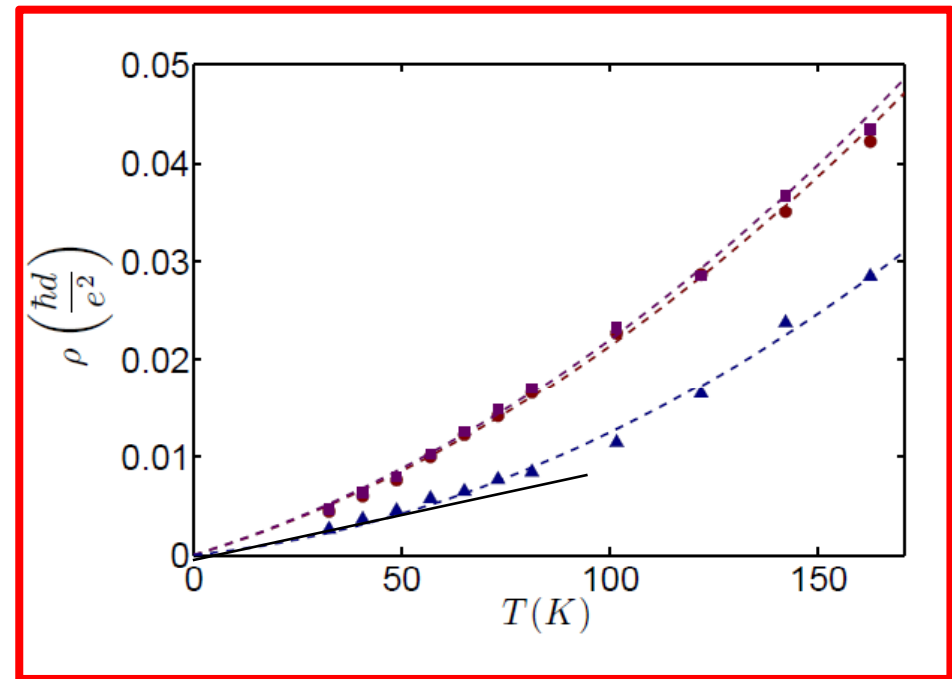
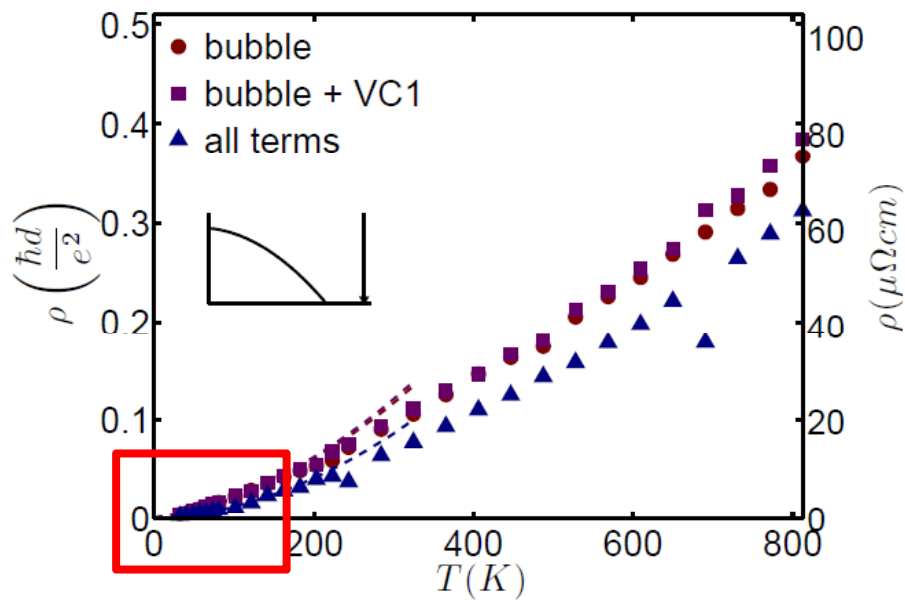
$$U = 6t, t' = -0.175t, t'' = 0.05t$$



$$\rho(T) = AT + BT^2$$

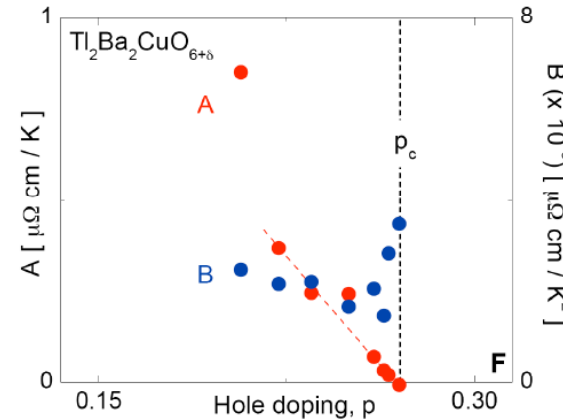
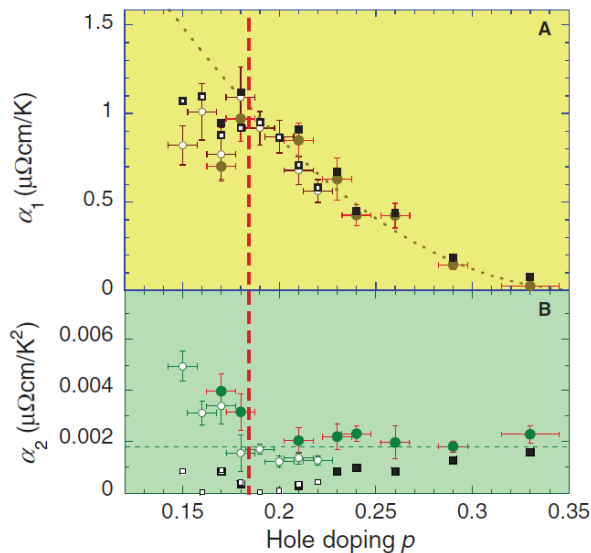
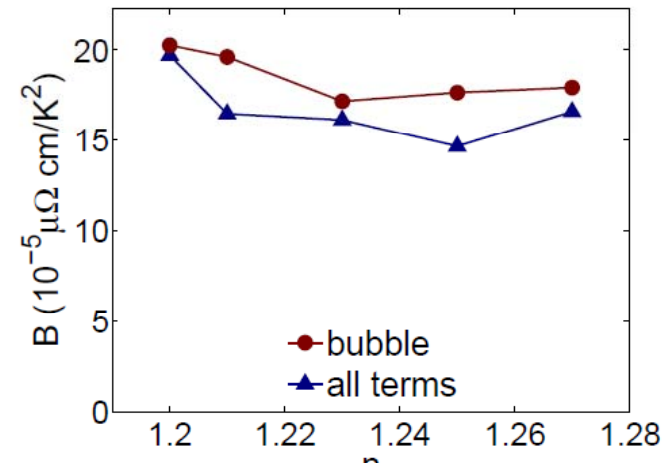
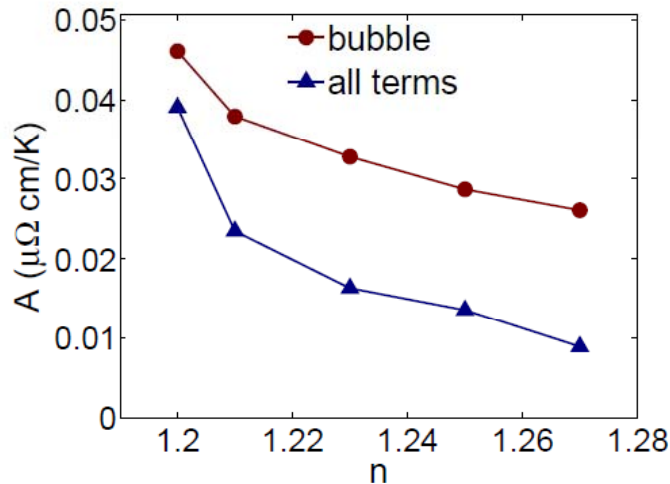
Right of the QCP

$$U = 6t, t' = -0.175t, t'' = 0.05t$$



Linearity for $n > n_c$ and T_c

Fitting $\rho(T) = AT + BT^2$ for all dopings:



Cooper et al.
Science **323**
30 (2009)

Doiron-Leyraud
et al. Phys. Rev.
B **80**, 214531
(2009)

Doiron-Leyraud et al. arXiv:0905.0964

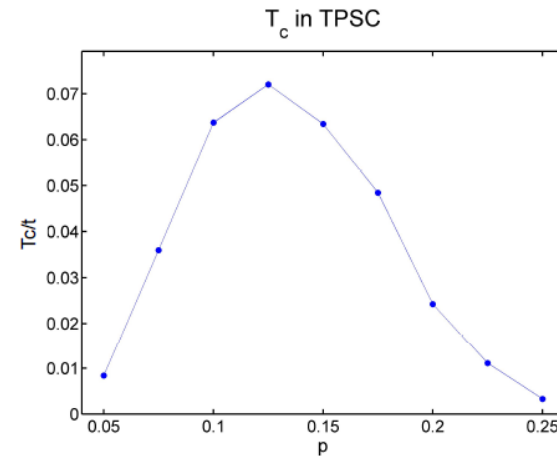
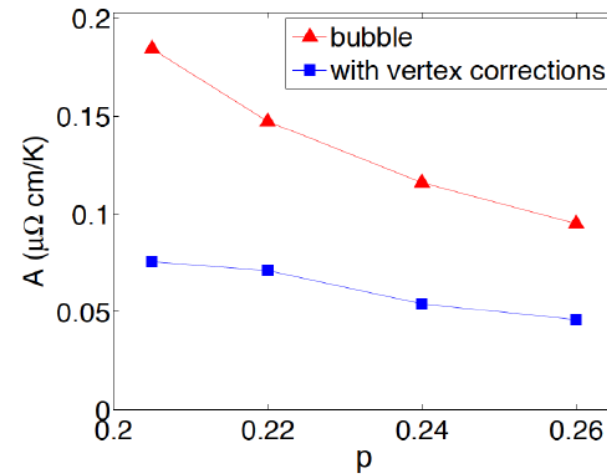
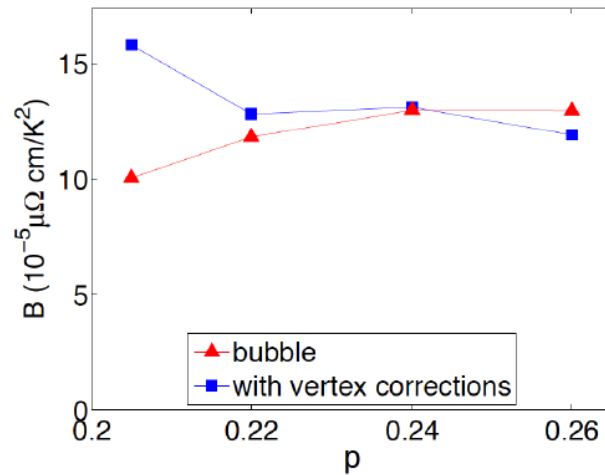


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Linearity for $n > n_c$ and T_c

$$U = 6t, t' = 0$$

By fitting $\rho(T) = AT + BT^2$ for all dopings:

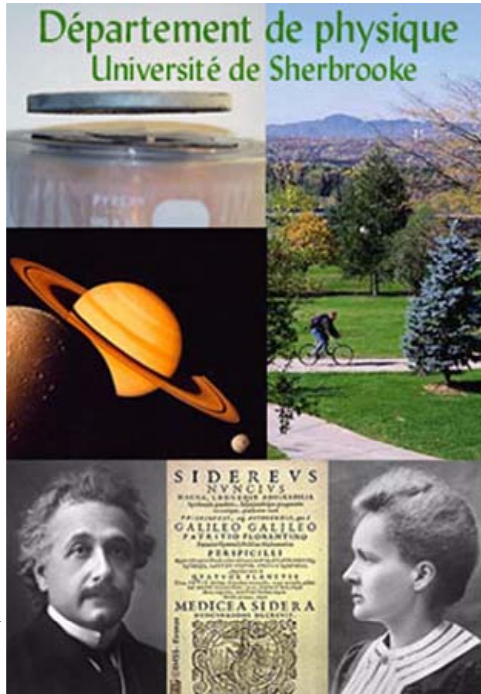


Conclusion

- Calculation: No-QP. Ioffe-Regel saturation
 - Hubbard bands necessary to violate MIR limit
- Vertex corrections are important close to half-filling.
 - They have non-universal effect
 - Less important away from QCP. Do not remove linearity (universal).
- Linear term decreases with n and disappears with SC
- Optical conductivity has mid-infrared peak.



André-Marie Tremblay



Le regroupement québécois sur les matériaux de pointe



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Thanks...

Merci